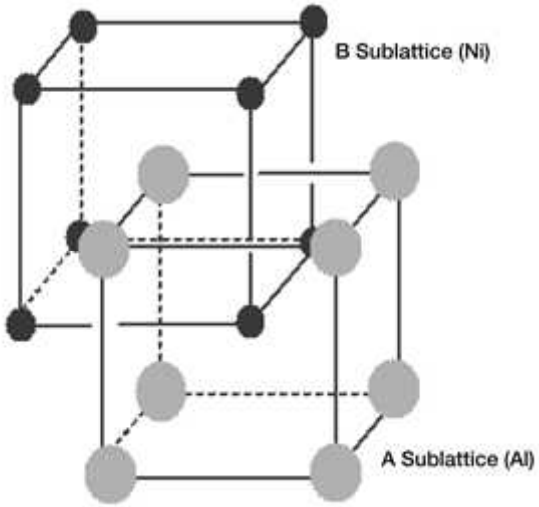
Alloy Design Data Generated for B2-Ordered Compounds



Structure of a B2 compound showing the two interpenetrating simple-cubic sublattices. In the case of stoichiometric NiAl, Ni atoms would occupy one sublattice and Al atoms the other.

Developing alloys based on ordered compounds is significantly more complicated than developing designs based on disordered materials. In ordered compounds, the major constituent elements reside on particular sublattices, see the drawing. Therefore, the addition of a ternary element to a binary-ordered compound is complicated by the manner in which the ternary addition is made (at the expense of which binary component). When ternary additions are substituted for the wrong constituent, the physical and mechanical properties usually degrade. In some cases the resulting degradation in properties can be quite severe. For example, adding alloying additions to NiAl in the wrong combination (i.e., alloying additions that prefer the Al sublattice but are added at the expense of Ni) will severely embrittle the alloy to the point that it can literally fall apart during processing on cooling from the molten state (ref. 1). Consequently, alloying additions that strongly prefer one sublattice over another should always be added at the expense of that component during alloy development. Elements that have a very weak preference for a sublattice can usually be safely added at the expense of either element and will accommodate any deviation from stoichiometry by filling in for the deficient component.

Unfortunately, this type of information is not known beforehand for most ordered systems.

Therefore, a computational survey study, using a recently developed quantum approximate method, was undertaken at the NASA Glenn Research Center to determine the preferred site occupancy of ternary alloying additions to 12 different B2-ordered compounds including NiAl, FeAl, CoAl, CoFe, CoHf, CoTi, FeTi, RuAl, RuSi, RuHf, RuTi, and RuZr. Some of these compounds are potential high-temperature structural alloys; others are used in thin-film magnetic and other electronic applications. The results are summarized in the following table. The italicized elements represent the previous sum total alloying information known and verify the computational method used to establish the table. Details of the computational procedures used to determine the preferred site occupancy can be found in reference 2. As further substantiation of the validity of the technique, and its extension to even more complicated systems, it was applied to two simultaneous alloying additions in an ordered alloy (ref. 3).

SITE OCCUPANCY PREFERENCE FOR TERNARY ALLOYING ADDITIONS IN VARIOUS B2-ORDERED COMPOUNDS

[Italicized data represent the sum total of previously realized information prior to this study.]

A(B,X) (A,X)B	Preference for sites in the A sublattice	Preference for sites in the B sublattice

	Strong	Medium	Weak	Very weak	Very weak	Weak	Medium	Strong
Ni(Al,X)					***Fe*** Ru	***Ta*** Cu ***Cr Mo Hf W Nb Zr***	***V***	Co ***Ti*** Si
(Ni,X)Al	Co Ru	Fe	SiCu	Cr Zr Hf	Ta Mo W Nb V Ti			
Fe(Al,X)			Ru ***Ni***	***Co***		Zr Si W Mo Cu	***Cr*** Nb Ta Hf	***V Ti***
(Fe,X)Al	Ru Ni	Co	Zr Hf Si Cu	Cr	W Mo V Ta Nb	Ti		
Co(Al,X)					Ni Zr Fe	W Hf Mo Cu Al Ta Ru Cr	V	Si Ti
(Co,X)Al		Fe Ni	Zr Hf Cu Ru	Cr	W Mo Ta V Nb Ti	Nb		
Co(Fe,X)				Si Co Cu V Mo W Ta Ni	Ti Al Hf	Ru	Cr	
(Co,X)Fe			Ni	Zr Si V Mo W Cu Ta	Ti Nb Al Hf Cr			
Co(Hf,X)					Fe Ni Ru W	Cr Mo V	Cu Ta Zr	Nb Si Ti
(Co,X)Hf	Ni Fe Ru		V Cr Mo W	Nb Ta	Cu Si Zr Al Ti			Al
Co(Ti,X)						W Ni	Cu Cr Al Mo Zr Hf	V Nb Si
(Co,X)Ti	Fe Ru	Al Ni	V Cr Cu Hf	Zr	W Si Mo Nb Ta		Ta	
Fe(Ti,X)				Co Ru	Ni	Al Cu Cr	Zr W Mo V Hf Ta	Si
(Fe,X)Ti	Ni Co Ru	Al	V Cr Hf Cu	Zr	Si Mo W Nb Ta		Nb	
Ru(Al,X)				Mo Ta Fe Cr	Zr Nb Hf Ti V Cu	Co Ni W		Si
(Ru,X)Al			Hf Ta Ti Nb Mo Ni Co Cu Zr Cr Fe	Si W V				
Ru(Si,X)				V Zr Hf Nb Ti Fe Cr Mo Ta		W Cu Ni Co	Al	
(Ru,X)Si	Fe	V Ti Mo Ta Cr	Cu W Ni Co Zr Hf Nb	Al				
Ru(Hf,X)				Ni Fe Co		Cr Mo W Cu	V Nb Ta	Si Al Zr Ti
(Ru,X)Hf	Ni Fe Co		Ta V Cr Mo W	Nb	Cu Si Al Zr Ti			
Ru(Ti,X)				Co	Fe Ni Cu	Cr	Hf Mo Al W Ta Nb	Si Zr
(Ru,X)Ti	Co Fe	Ni	V Cr Cu Hf Al	Zr Si	Mo Nb W Ta		V	
Ru(Zr,X)				Ni	Cr	Co Cu Fe Mo V W Nb	Ta Si	Hf Ti Al
(Ru,X)Zr	Ni	Ta Cr	Cu Fe Si W V Mo Nb	Ti Co Al Hf				
Ru(Ti,X)				Co	Fe Ni Cu	Cr	Hf Mo Al W Ta Nb	Si Zr
(Ru,X)Ti	Co Fe	Ni	V Cr Cu Hf Al	Zr	Si Mo W Nb Ta		V	

The information in this table can be used to guide future alloy design programs involving any of these systems. Significant savings in time, money, and effort should result because the focus will be on the most energetically stable compositions. In addition, the methodology can handle other alloys and types of ordered structures.

Find out more about this research:
International Computational Material Science Consortium http://www.icmsc.org/
Ronald D. Noebe http://www.grc.nasa.gov/WWW/MDWeb/People/20NRD.html

References

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